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CompReact: Compositional Simulation of Reactive Transport in CO_2 Storage

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Carbon capture and storage (CCS) is a key strategy for reducing greenhouse gas emissions and mitigating climate change. The process involves capturing CO_2 from various sources and storing it in geological formations, but the long-term stability and safety of CO_2 storage sites are not yet fully understood. The CompReact project, funded by Innovation Fund Denmark under the INNO-CCUS research partnership, aims to improve our understanding of CO_2 storage by developing advanced simulation techniques that can capture the complex chemical reactions that occur when CO_2 is injected into subsurface reservoirs.

The project focuses on developing high-resolution numerical models that can simulate how CO_2 interacts with the rock matrix, fluids, and other geochemical components in the storage reservoir. The models account for the transport of fluids, gases, and heat, as well as the chemical reactions between CO_2 and the minerals in the reservoir. The researchers plan to develop a next-generation compositional CO_2 storage simulator with multiphase geochemical reactions that is applicable to various geological reservoir types, including aquifers and depleted petroleum reservoirs, and dramatically improved in terms of efficiency and robustness.

To achieve this, the researchers plan to utilize novel RAND-based multiphase reaction algorithms that have recently been developed at DTU. The algorithms treat phase and chemical equilibrium simultaneously and are particularly suited to situations with many phases and reactions, such as CO_2 storage. The developed simulator will be able to handle both near-wellbore and reservoir-scale simulations during the injection and post-injection periods, with a general non-isothermal formulation to account for local operational issues.

The project involves two work packages, focusing on the development of a highly-efficient compositional reactive simulator and large-scale simulation coupled with GEOSX. The new GEOSX simulator will be applied to long time-scale post-injection simulations with coupled geomechanics, allowing for the analysis of pressure and stress variation and CO_2 plume development. This project is and the coupling of the two work packages is a collaboration with Stanford University.

In summary, the CompReact project aims to develop a highly efficient and reliable CO_2 storage simulator with multiphase geochemical reactions that will be applicable to various geological reservoir types. The novel RAND-based algorithms developed at DTU will be utilized to provide a new formalism for compositional CO_2 storage simulation with multiphase reactions. The coupling with GEOSX will create synergy based on complementary expertise, allowing for the analysis of pressure and stress variation and CO_2 plume development during long-term simulations. This project will significantly contribute to technical risk assessment and support the realization of a sustainable carbon-neutral energy system.